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Factors driving refinery CO_2 intensity, with allocation into products: comment

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Abstract
Purpose Recently, using a long-run refinery simulation model, Bredeson et al. conclude that the light transportation fuels have roughly the same CO_2 footprint. And, any allocation scheme which shows substantial difference between gasoline and diesel CO_2 intensities must be seen with caution. The purpose of this paper is to highlight the inappropriate modeling assumptions which lead to these inapplicable conclusions into the current oil refining context.
Methods From an economic point of view, optimization models are more suitable than simulation tools for providing decision policies. Therefore, we used a calibrated refinery linear programming model to evaluate the impact of varying the gasoline-to-diesel production ratio on the refinery's CO_2 emissions and the marginal CO_2 intensity of the automotive fuels.
Results and discussion Contrary to Bredeson et al.'s conclusions, our results reveal that, within a calibrated optimization framework, total and *per*-product CO_2 emissions could be affected by the gasoline-to-diesel production ratio. More precisely, in a gasoline-oriented market, the marginal CO_2 footprint of gasoline is significantly higher than diesel, while the opposite result is observed within a diesel-oriented market. These two scenarios could reflect to some extent the American and the European oil refining industry for which policy makers should adopt a different per-product taxation policy.
Conclusions Any relevant and economic ground CO_2 policies for automotive fuels should be sensitive to the environmental consequences associated with their marginal productions. This is especially true in disequilibrium markets where the average and marginal reactions could significantly differ. Optimization models, whose optimal solution is fully driven by marginal signals, show that the refinery's global and/or per-product CO_2 emissions could be affected by the gasoline-to-diesel production ratio.

Keywords Diesel production · Gasoline production · Linear programming · Marginal CO_2 footprints · Oil refining

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1 Introduction

Recently, in a journal article, Bredeson et al. (2010) published a very interesting analysis of the CO_2 intensity of petroleum products at the gate of oil refineries. Using the Shell refinery simulation model, they evaluated the consequences of varying the crude diet, the gasoline-to-diesel production ratio, and the complexity of the refineries on their CO_2 emissions and their products' CO_2 footprint.

We fully agree with the authors conclusions concerning their first and third scenarios: the refinery energy use and CO_2 emission increase by running heavier crude and by increasing the complexity of the refinery, i.e., adding a coker or other residue reduction process units. Their analysis about the key role of the reformer unit as an energy/CO_2-equalizing device seems exact to us and also important for a better understanding of the different estimations of the gasoline CO_2 footprint in the literature (e.g., Furoholt 1995; Palou-Rivera et al. 2011; JRC/IES, EUCAR, CONCAWE (JEC) 2011; Wang et al. 2004). However, we must disagree with some conclusions on the impact of varying the gasoline-to-diesel production ratio on the total and per-product CO_2 emissions and the related policy

recommendations. Throughout this paper, we only consider this scenario.

The refinery simulation model used by Bredeson et al. is fully adjusted to the demand market and operates at its natural capacity; and the production ratios fall within “normal range” of the refinery flexibility. Based on these strong assumptions, the authors conclude that (a) the light transportation fuels have roughly the same CO_2 content and (b) the refinery's CO_2 emissions are practically independent of the gasoline/diesel production ratio. Although they themselves admit that producing out of normal ranges could negate these conclusions (p. 822), their general recommendations to policy makers is to see with caution any allocation scheme which shows substantial difference between gasoline and diesel CO_2 intensities. However, and as our main remark, we must note that neither the European nor the American oil refining industry satisfies Bredeson et al.'s theoretical assumptions. The structural market disequilibrium in both industries has led their gasoline-to-diesel production ratio out of the normal ranges relative to their respective refining scheme. As a consequence, the authors' recommendations (on this part) become of little use and misleading for policy makers.

2 Marginal CO_2 footprints and policy analysis

2.1 Refinery optimization versus simulation models

In Bredeson et al.'s context, the consequential life cycle assessment (CLCA) is the approach used to estimate the CO_2 consequences of modifying the production ratio between gasoline and diesel at the refinery gate (for a detailed discussion about CLCA methodology, see for instance Tillman 2000 and Zamagni et al. 2012). Within a given refinery scheme, total CO_2 emissions are a function of the crude slate's properties and the quantities and specifications of the refined product outputs. So, varying the gasoline-to-diesel production ratio can affect the refinery's CO_2 emissions through a wide range of feasible possibilities. Refinery simulation models could provide any of these technically feasible solutions based on how the streams are internally routed and how the process units' operating parameters are manually set up (in response to a change). Most often, these configurations are driven by the user's experiences and her day-to-day available information and, thus, may not always be optimal. Contrary to simulation models proposed by Bredeson et al. (p. 819), we would suggest using the well-established and calibrated refinery linear programming (LP) models that would directly provide the unique processing operations leading to an optimal solution in a cost-efficient sense. By construction, LP models endogenize simultaneously the economic signals (market prices, environmental taxes, opportunity costs, and substitution effects) and the refining processing mechanisms. Coupling these two impacts is essential; otherwise, the economic and ecological interdependencies would be neglected and might cause policy failures (Bartelmus 2008). Finally, and as opposed to simulation tools which are usually used to schedule the daily-based operations of an oil refinery, we believe that optimization models are more suitable to provide economic policies (see Pinto et al. 2000 for a discussion about the optimization planning and scheduling refining models).

In any petroleum refinery LP model, an explicit emission balance equation can be set in order to capture all CO_2 emissions of refinery activity. These emissions are mostly generated from burning fuel gas, liquefied petroleum gas, liquefied fuel, coke of the catalytic cracker, and imported natural gas to provide the (fix and variable) utility requirement of the process units. Furthermore, hydrogen production units also contribute to the refinery's CO_2 emissions. The well-known characteristic of a cost minimization LP model is to convert the above input-related CO_2 emissions into a partially product-related CO_2 emission based on a marginal principle (for mathematical proofs, see Tehrani Nejad 2007). Explicitly, at the optimal solution of a cost minimization LP model, the positive basic CO_2 variable is given as a linear function of the active constraints,

$$E = \sum_i \alpha_i \ b_i \ + \ \sum_j \gamma_j \ f_j \tag{1}$$

where E corresponds to the amount of CO_2 that must be released for satisfying the product output b, at the given refinery complexity, the short-run process unit capacity and logistic constraints f, and the market input–output prices. In relation (1), the product-related coefficient α_i measures the marginal CO_2 intensity of the ith oil product extracted from a cost-efficient solution. At the optimal solution, these marginal coefficients are computed by tracking the CO_2 emissions through individual process units and include the interdependencies among inputs and outputs simultaneously (i.e., the boundary expansion related to a marginal change at the refinery gate). Therefore, the marginal CO_2 footprints α_i are not resultant of any ad hoc allocation rule and thus satisfy the CLCA recommendations. These marginal signals are the only economic ground indicators in joint production systems such as petroleum refineries. Similarly, the process-related coefficient γ_j refers to the marginal CO_2 intensity of the jth process unit. Comparing to simulation models, we believe that the marginal-based CO_2 footprints in relation (1) provide more relevant information for decision making (for further discussion about the LP-based data in LCA studies, see Azapagic and Clift 1998, 1999, 2000 and Tehrani Nejad 2010).

2.2 Global versus composition effects

Bredeson et al. argue that “if the refinery runs showed no difference in total refinery CO_2 emissions as the gasoline-to-diesel ratio was varied, then the CO_2 intensity of those two fuels should be same” (p. 819). We hold an opposite point of view. In relation (1), depending on the optimal production plan, the marginal CO_2 intensities α_j and γ_j can be positive, negative, or zero. Therefore, we can think of a scenario where the “composition” of the equation can change without affecting the “global” CO_2 emissions, *E*. For instance, and in line with the authors' analysis (p. 820), the refinery production shift from gasoline to diesel would increase the H_2 requirement due to further (hydro)-cracking and hydro-desulfurization processes. In reality, it is likely that this additional H_2 needs to be satisfied by the H_2 supply plants (e.g., a steam reformer) which would lead to an increase in the refinery's CO_2 emissions. But we can also assume that a sufficient availability of the reformer unit and relevant input–output price ratios would enable the reformer to produce this additional H_2, leading to a constant use of the other H_2 plants which are very CO_2 intensive. Under these assumptions, indeed, the overall CO_2 emissions of the refinery might not change very much. However, increasing the H_2 production from the reformer leads intrinsically to increase gasoline output that we intend to reduce by assumption. Borrowing the authors' vocabulary, this highlights the not “on-purpose” nature of the last tons of gasoline in this example. Due to the marginal rate of technical transformation, LP models naturally track these interdependencies and readjust accordingly the marginal CO_2 intensities of the outputs. Note that these adjustments are intrinsic to LP models and do not require any ad hoc hydrogen transfer term as is suggested by Bredeson et al. We believe that policy makers should be also concerned with this composition effect, especially when they seek to define CO_2 taxes per product. Moreover and depending on the economics, optimization models might also vary significantly the total CO_2 emissions when the gasoline-to-diesel ratio is modified (see Section 3).

2.3 How relevant are the adjusted capacity models?

On several occasions, Bredeson et al. rightly recommend that the calculated CO_2 intensity of petroleum products should be consistent with the actual refinery behavior. Petroleum refiners are economic agents whose production behavior is driven by market signals subject to their production constraints. With this recommendation in mind, we are rather surprised to read that they removed all capacity constraints, and “the process unit throughputs are allowed to vary as needed.” Their justification is “had that not been done, the results would have been strongly and inappropriately biased by internal constraints” (p. 820).

We admit that the authors' case studies would have been most likely infeasible within a fixed set of capacity constraints. In such cases, however, investment models should be used in which (realistic) additional processing capacity is permitted within a cost. Otherwise, removing all capacity constraints implies that refineries are operating at optimal capacity and are fully adjusted to their market demands. This might make sense when considering the global refining industry at world scale. However, the products' CO_2 taxation policies are far from being homogenous and are more concerned with the US and the European countries whose refining industries are suffering to match the strong changes in their domestic demand trends. For instance, at least for the past 15 years, the gasoline demand is in structural decline in Europe. For the time being, European gasoline surplus is exported to the USA, Africa, and the Middle East. But this “vital” export flows for Europe are likely to be affected by the increases in Middle Eastern and Indian refinery capacities as well as the use of bio-ethanol in gasoline. Moreover, increasing product volumes in export markets will have the effect of putting downward pressure on prices and thus reducing the economic incentive for further investments (Purvin & Gertz 2008). On the other hand, and despite some additional hydrocracking units, European refineries are significantly short in diesel (and middle distillate) production. This disequilibrium can be illustrated by the gap between the demand and supply gasoline/diesel in Europe in 2010, which were respectively equal to 0.5 and 0.8. The same ratios for the USA were, respectively, 3 and 2.7 (IFPEN internal report from IEA 2012 and KBC 2012). In such circumstances, Bredeson et al.'s capacity relaxations are a serious handicap for drawing the following general (and misleading) recommendation: “any allocation scheme which shows CO_2 intensities of gasoline and distillate are substantially different must be seen with caution” (825).

3 Case study

The objective of this section is to reevaluate the impact of varying the gasoline/diesel production ratio on the total CO_2 emissions of the refinery and the marginal CO_2 intensity of the automotive fuels. To this end, a real-type investment LP model is used.

3.1 General description of the model

The LP refinery model used here has been developed by *IFP Energies nouvelles* and corresponds to a typical European refinery of 7.5 million metric tons/year of crude oil processing capacity. The important processing units are an atmospheric and a vacuum distillation, a catalytic reformer, an isomerization unit, a vacuum gas oil (VGO) hydrodesulfurization (HDS),

a fluidized catalytic cracking (FCC), an alkylation unit, a hydrocracking unit HCK, three gas oil HDS units, a visbreaker, and a sulfur plant. All process units are limited by their installed capacity. Further (realistic) investment is permitted within a cost.

The crude slate is reduced to Brent, Arabian Light, and Arabian Heavy. This simplified model (with 650 constraints and 1,700 variables) can also import natural gas, hydrogen, and atmospheric residue (as conversion feedstock). All input prices correspond to their average price of 2010. The oil product categories considered are propane, butane, naphtha, gasoline (domestic and export grades), jet fuel, diesel, heating oil, heavy fuel oils with 1and 3.5 % mass sulfur contents and bitumen. The refiner's objective is to satisfy a net production level (i.e., domestic demand plus the net exchange) of these petroleum products at minimum cost (see Tehrani Nejad and Saint-Antonin 2008 for further details).

As shown in Table 1, two scenarios S1 and S2 are studied. Scenario S1 is calibrated to the European base year 2010, with, in particular, a representative gasoline-to-diesel production ratio of 0.8 (see Section 2.3). Within the same refinery scheme, the gasoline/diesel production ratio is increased from 0.8 to 1.1 in S2. Although this ratio is still below the US observed value of 2.7 for the same year, S2 is a suitable candidate to mimic the CO_2 footprint of automotive fuels in the US context. This ratio gap is simply due to the choice of keeping the same refining scheme with a hydrocracker and a visbreaker unit (instead of a coker). This assumption would isolate the impact of the production ratio from the refining scheme and would lead to more comparable results to Bredeson et al.'s second scenario.

4 Results and discussions

At the optimal solution, the total CO_2 emissions and marginal CO_2 intensities are extracted from relation (1). A sensitivity analysis is performed to guarantee the stability of the marginal CO_2 footprints. The main results are summarized in Table 2. The following remarks are in order. First, within almost the same global input (−2.4 %m) and output (−1.3 %m) levels, increasing the gasoline/diesel ratio decreases the total CO_2 emissions by more than 11 %. This significant CO_2 reduction is explained as follows. Decreasing the diesel production (−30 %m) in S2 reduces the HCK and the VGO HDS feeds by 25 and 37 %m, respectively. Moreover, the incorporation of the imported atmospheric residue to the FCC feed drops from 64 to 32 %m, enabling to produce directly more gasoline with less sulfur content. These sole adjustments significantly reduce the hydrogen requirement. On the other hand, the increased gasoline production in S2 leads to an increase in the reformer operation by 20 %m (expansion capacity). Finally, this leads to a reduction of the hydrogen plant operations (−24 %m) which are very CO_2 intensive. The excess hydrogen (with null CO_2 content) is increased from 2 to 4 % and is burnt as refinery fuel. Finally, the high sulfur liquid fuels are no longer burned but exported. All these *optimal* substitutions imply a consequent decrease in the refinery's CO_2 emissions (−11 %).

Second, the hierarchy between the marginal gasoline and diesel CO_2 footprint is reversed between S1 and S2. In S1, diesel represents almost 31 % of the global production of the refinery. In this case, representing the European refining context, the reformer unit operates at full capacity not for the gasoline demand but in order to meet the important hydrogen requirement of the refinery (taking into account the actual gasoline export capability of our typical European refinery model). The LP mechanism is sensitive to these interdependencies, and the reformer unit (and ultimately gasoline) is not wrongly penalized for its intensive operation. On the other hand, S2 tends to reflect to some extent the American scenario in which the gasoline fraction has expanded beyond its optimum balance with diesel yield (within the given refinery scheme). As implied from Table 2, the per-product CO_2 taxation policy must be different between a diesel- and gasoline-oriented market. For instance, encouraging the European domestic gasoline demand by revising the existing tax policy (inspired by a lower marginal CO_2 footprint) might help to correct the disequilibrium of the European automotive fuels market. The US context, obviously, needs the reversed signal.

Table 1 Net production

	S1	S2
Propane	0.176	0.178
Butane	0.104	0.083
Naphtha	0.264	0.301
Gasoline (local)	1.849	2.000
Gasoline (export)	0.000	0.085
Jet fuel	0.339	0.339
Diesel	2.283	1.620
Heating oil	0.803	0.853
Fuel oil 1 %	0.500	0.500
Fuel oil 3.5 %	0.700	0.962
Bitumen	0.200	0.200
Sulfur	0.068	0.068
Total	7.286	7.189

Unit, metric ton per year

Table 2 Total and per-product marginal CO_2 emissions

	CO_2 emissions (Mt)	Gasoline footprint (t CO_2/t)	Diesel footprint (t CO_2/t)
S1	1.59	1.24	1.97
S2	1.41	2.45	0.58

Third, the modeling framework and system boundary used in this paper make the above results comparable with those obtained in Bredeson et al.'s second scenario. However, in the existing LCA database, there exist other different evaluations for the automotive fuels' CO_2 footprint; see, for instance, Gabi6 (PE International 2007), Ecoinvent (Jungbluth 2007; Jess 1996), and JEC (2011). Note that any direct comparison between our findings and those reference results, which are also different between them, must be done with caution. In effect, the regional specificities, the refinery scheme and its complexity (as shown by Bredeson et al.), the aggregation level of information, the type of question raised, the allocation criteria, the specific treatment for hydrogen, and many other technical issues make this comparative study nontrivial. Such a discussion is very important and still missing in the LCA oil refining literature.

5 Conclusions

Any CO_2 allocation scheme should reflect as closely as possible the underlying difficulties of a production process and be sensitive to both global and composition effects. In this paper, using a short-run optimization model, we showed that total and per-product CO_2 emissions of a refinery could be affected by the ratio of gasoline to diesel product. Contrary to Bredeson et al.'s recommendation, we believe that the per-product CO_2 taxation policy must be different between a diesel- and gasoline-oriented market.

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